HTAC: An atomic multiplet code for the calculation of various atomic properties

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Abstract
We describe an atomic multiplet code (HTAC) for the calculation of various atomic radiative processes, including energy levels, oscillator strength, radiative transition rates, mixing coefficients for any rank of mutipole transitions, and other quantities.

1. Introduction
User interfaces are becoming more and more complex as the underlying applications add more and more features. Although most people use only a small subset of the functionalities of a given program at any given time (J. McGrenere et al., 2002). Consider the FAC code (Gu, 2008) as an example. This code is a relativistic configuration interaction atomic code, and uses the distorted-wave approximation to treat electron-ion collision processes. It has two interfaces SFAC and PFAC. The flexibility of the FAC is realized when the Python interface PFAC is used. Moreover, to use the PFAC interface, user needs to be familiar with the Python scripting language in order to compose the input file. Therefore, the computation task will be completed by programming in the scripting language Python. Theses python scripts will make it easy to include any specified function from the FAC library in the input file to be exported through several Python modules. However, using the flexible PFAC is limited to those who are familiar with Python scripting language, which is not commonly used by public. In the meantime, trained interface designers cannot always foresee how a software package is going to be used in practice, especially if the package is used by a large variety of different users this makes creating a flexible user interfaces a major challenge. From this point, it is clear that there is a real need for having an easy to use atomic code encompasses FAC strengths and enhanced with extra capabilities.

This paper introduces the first version of Hamasha-Tahat Atomic Code (HTAC) (Hamasha and Tahat, 2009) .This code is a utility program working under Windows platform with a flexible Graphical User Interface (GUI) that supplies a number of basic functionalities to facilitate the use of some existing atomic codes. It is developed primarily to support the use of the first part of the latest version of the FAC package that can be obtained from (URL:http://sprg.ssl.berkeley.edu/~mfgu/fac/fac.tar.gz). It provides users with a number of documents. They are included in the doc folder of the distributed package including five papers that describe the detailed atomic physics model of the code. One of them entitled "The Flexible Atomic Code: I. Atomic Structure" provides a full description of the theoretical background related to the atomic structure calculation and bound-bound processes that based on the Configuration Interaction Method (CIM) in fully relativistic approach. HTAC can easily be modified to support the other parts of FAC as well. Furthermore; HTAC provides viewing and plotting capabilities and enables researchers to run the code even if they are not familiar with computation theories or programming languages. The rest of the paper is organized as follows. In the next section, we present a description of the individual software components and a brief overview of the software structure .In section three we present the way of running the atomic structure program, input files, output files, flexibility, validity, plotting capability, error massages and the future work of HTAC. Additionally, section three presents several examples and results comparisons to illustrate the concepts followed by the conclusion. Finally the entire package is publicly available upon request to the author and it is a step forward to bring detailed atomic model accessible to a wide community of laboratory and astrophysical plasma diagnostics.

2. The Software Structure

2.1. Description of the Individual Software Components:

HTAC used free software's obtained from www.cygwin.com which included GCC, GFortran (c/c++/f77 compiler), tk/tcl and python interpreter. HTAC is written mainly in Python and some of its GUI extension modules like "TKinter" and its extension "pmw" besides using the dynamic language TCL. HTAC used "The numeric python module" for defining a multi-dimensional array and useful procedures for Numerical computation functions in PFAC library. C, C++ and FORTRAN were used in the modifications of numerical procedures, such as bugs fixing and inconsistent behavior of library files. Figure 2.1. shows the interconnection of HTAC and PFAC and their programming languages.

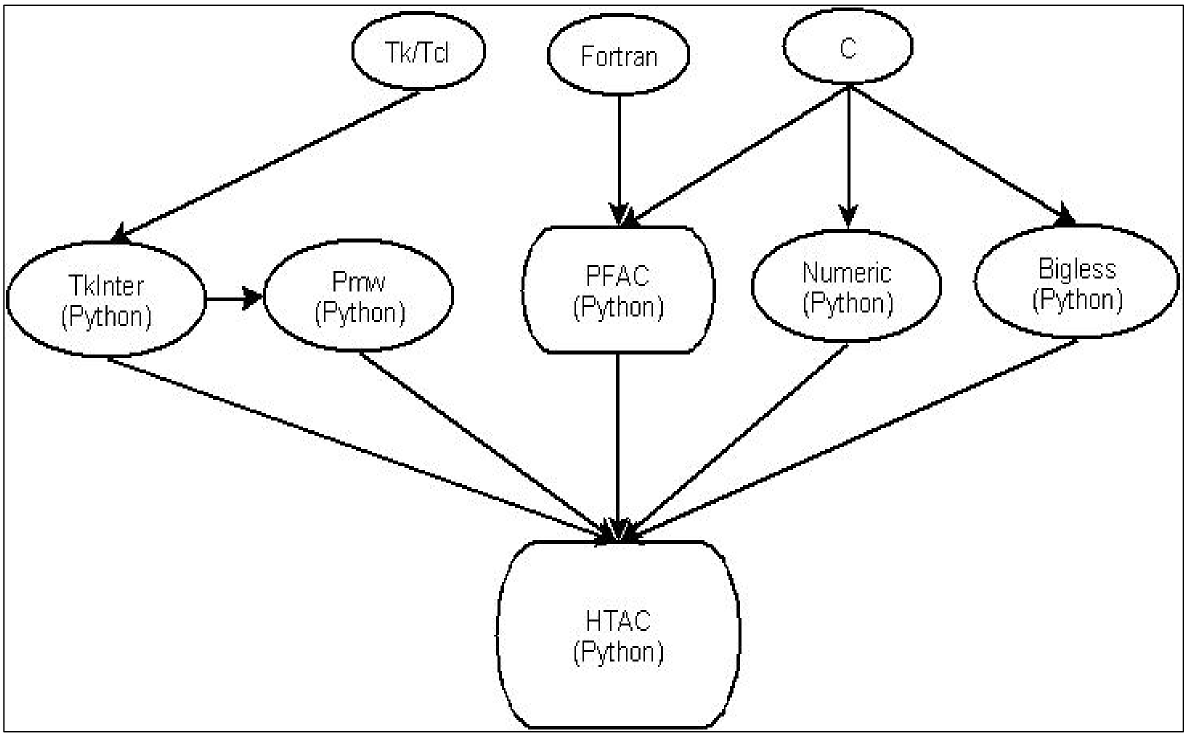


Figure 2.1. Interconnection of HTAC and PFAC and their programming languages. Many FORTRAN 77 subroutines were retrieved from Net lib repository (www.netlib.org) and used in FAC package, as well as several programs from Computer Physics Communications Program Library at www.cpc.cs.qub.ac.uk.

2.2. A brief overview of the software structure

This is the first version of HTAC .It consists of the (atomic structure program of FAC) that designed to obtain energy levels, oscillator strengths, radiative transition rates, wave function, mixing coefficients and reduced multipole matrix elements for any rank of mutipole transitions (E1, E2, E3, M1, M2, M3,) and a variety of other atomic quantities. The atomic structure calculations based on two advanced methods in atomic physics, the Configuration Interaction Method (CIM) and the new modified Many Body Perturbation Theory (MBPT). (Gu, 2005; Gu et al., 2006a; Gu et al., 2006b). The CIM works for systems with many valence electrons but can not accurately account for core-valence and core-core correlations. The MBPT can not accurately describe valence-valence correlation. Therefore, two methods are combined to acquire benefits from both approaches. Figure 2.2.1 shows the location of the program (atomic structure) in HTAC.

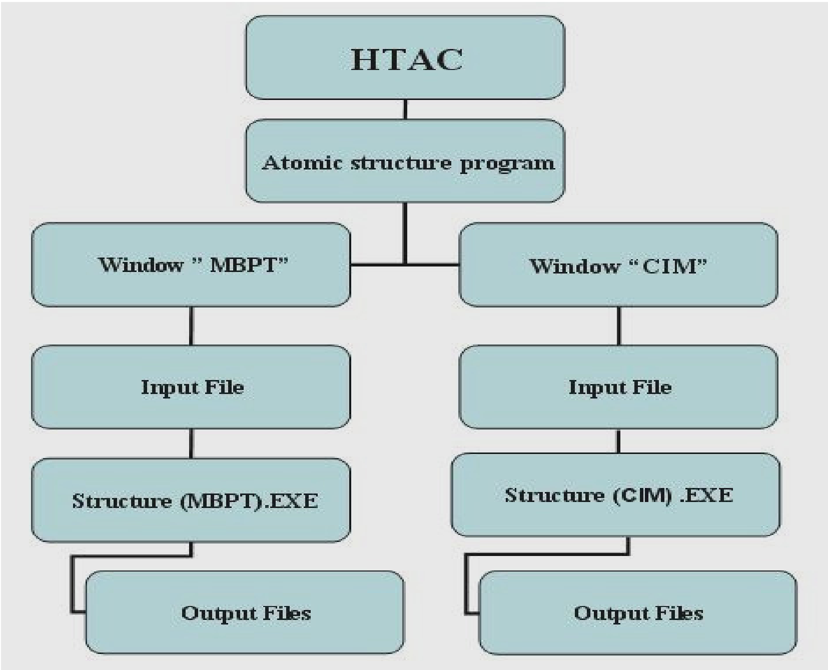


Figure 2.2.1. The structure of the 'atomic structure' program in HTAC.

3. Running the Atomic Structure Program

3.1. Atomic Structure Main Panel

To run the atomic structure program, the user clicks on "Atomic calculations" button from HTAC standard toolbar, and then a window pops up showing "Atomic structure program" main panel like the one illustrated in figure 3.1.1. which defines the input file.

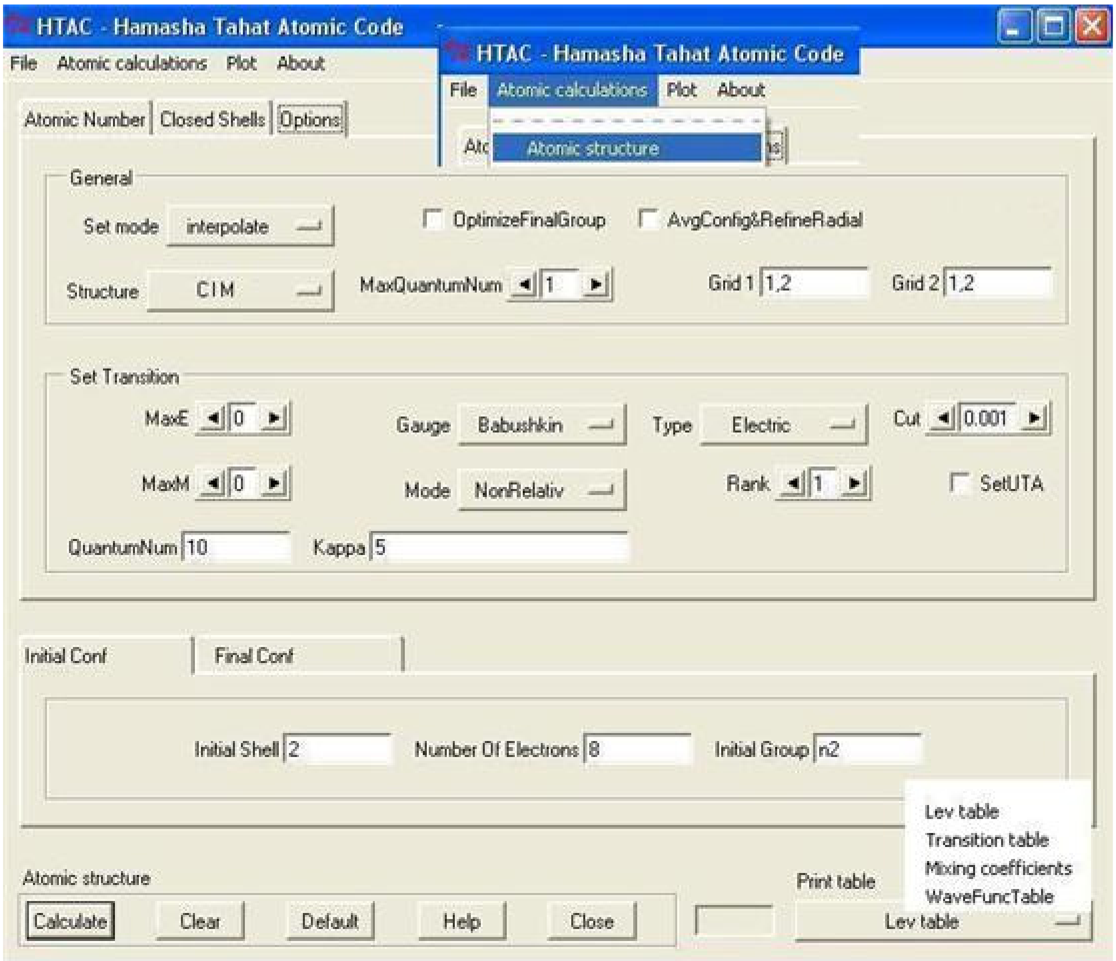


Figure 3.1.1. Main panel of HTAC, the atomic structure program, the atomic structure menu and the print table bar.

3.2. HTAC Input and Output Files

One of the most tedious steps of an atomic structure calculation is usually setting up the input file. Table (3.2.1) presents the way of composing the input file by using the PFAC interface of the FAC code which is available in the FAC manual. It is clear that user needs to write the required python scripts in order to set the atom, determine the closed shells, electronic configuration plus calling some specified functions for the calculation of energy levels and radiative transition rates which seems difficult and time consuming.

```
1: from pfac import fac
2: fac.SetAtom ('Fe')
3: # 1s shell is closed
4: fac.Closed ('1s')
5: fac.Config ('2*8', group = 'n2')
6: fac.Config ('2*7 3*1', group = 'n3')
7: # Self-consistent iteration for optimized central potential
8: fac.ConfigEnergy (0)
# The configurations passed to OptimizeRadial should always
# be one or two of the lowest lying ones. If you need more highly
# excited levels, such as n=4, 5, 6... do not put them into
# OptimizeRadial.
9: fac.OptimizeRadial (['n2'])
10: fac.ConfigEnergy (1)
```

```
11: fac.Structure ('ne.lev.b', ['n2', 'n3'])
12: fac.MemENTable ('ne.lev.b')
13: fac.PrintTable ('ne.lev.b', 'ne.lev', 1)
13: fac.PrintTable ('ne.lev.b', 'ne.lev', 1)
14: fac.TransitionTable ('ne.tr.b', ['n2'], ['n3'])
15: fac.PrintTable ('ne.tr.b', 'ne.tr', 1)
```

Table 3.2.1. FAC input file for the calculation of Ne-like iron energy levels and radiative transition rates between n = 2 and n = 3 complexes.

HTAC simplifies composing this input file by creating a system file that contains all information on the atomic configuration and geometry of a system. Various ways of visualization are supplied to document or check the created atomic configuration that makes use of the program FAC .The system file is independent of the program package used and can be stored and retrieved again later. Calling the ' structure program' allows to set up specific input files using the information stored in a system file. In addition program execution can be prepared and initiated in various ways by using the "option" tab. The resulting output data can be further processed using the program plot to create graphics files. Moreover, HTAC is still under construction, where graphics are of no use at this stage, but may be useful when the scattering parameters are added. The HTAC main panel allows defining the configurations of the initial and final states of the transition. The user has three options to define the input data:

1. Default data is provided through a built-in default input file named "structure. In". It contains the required data to obtain energy levels and radiative transition rates for Ne-like iron ion, which has the initial configuration $1s^2$ $2s^2$ $2p^6$, the transition between groups (or complexes) n=2 and groups n=3. The final configuration $1s^2$ $2s^2$ $2p^5$ $3*l$, the shell 1s is a closed shell. This option is available as a tutoring example through the "help" button in HTAC main panel of atomic structure program (Figure 4).

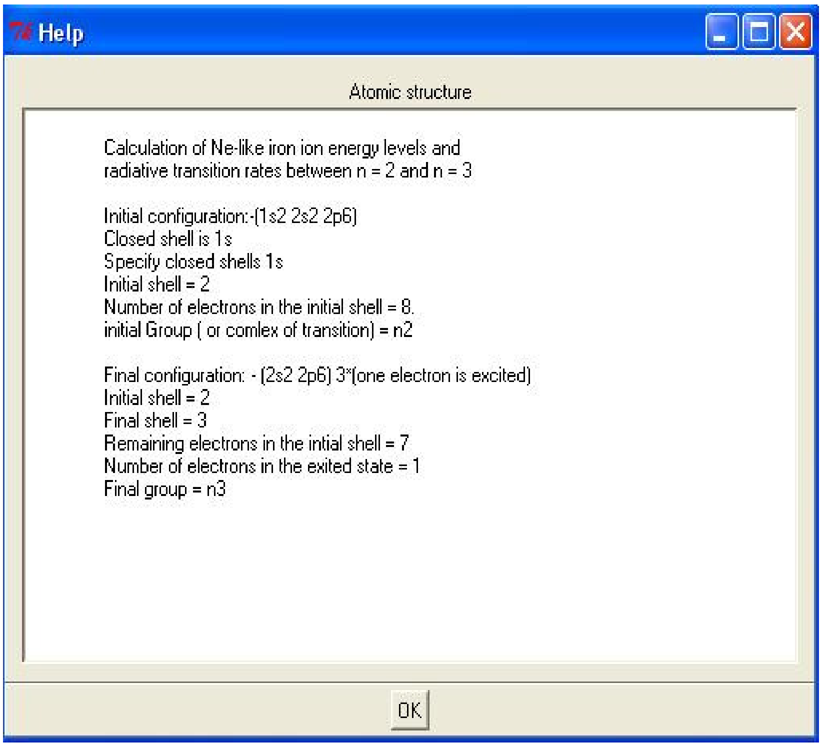


Figure 3.2.1. The help window demonstrates the input file for Ne-like iron ion

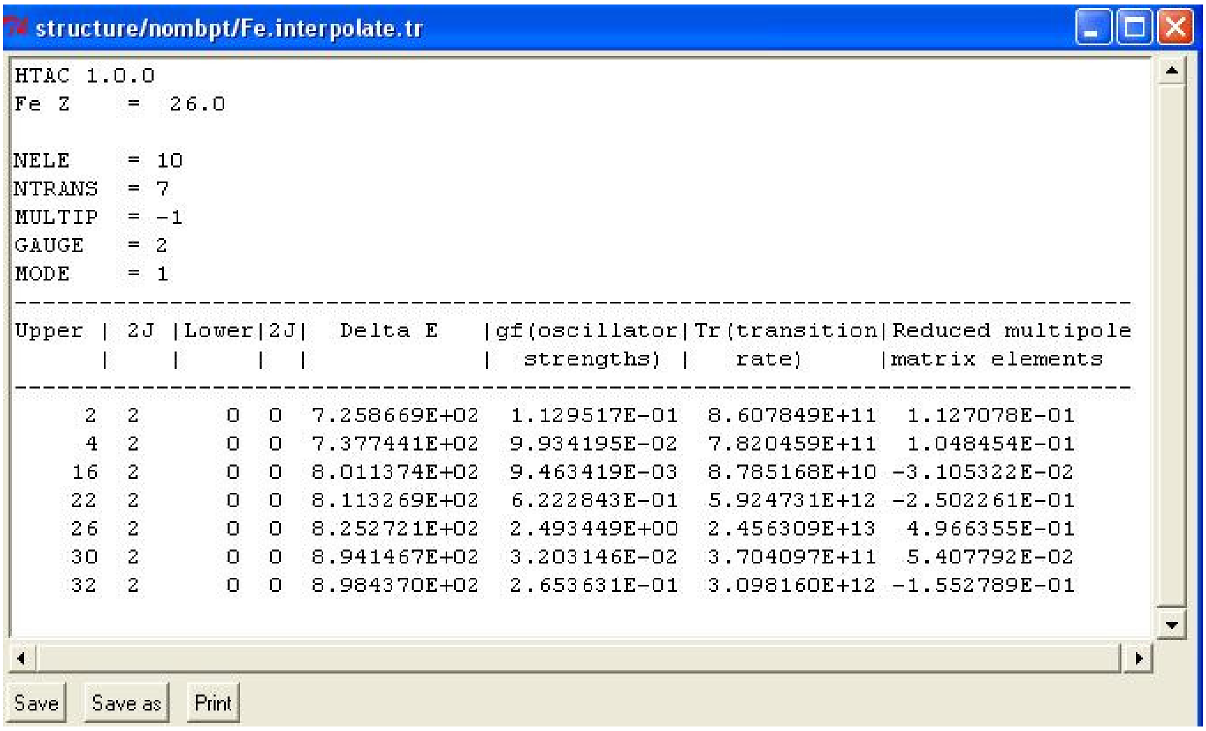
2. A comprehensive database for 100 elements and their characteristics including atomic number, closed shell, initial configuration, final configuration and other important information. HTAC user may import input files through the "Open" button in the file menu to be assigned to specialized fields in the main panel of the structure program.
3. Own data can be defined by the user in order to build the input file. Before constructing the own input data file, the user must select the button "clear" to empty all fields in the main panel then to identify the desired electronic configurations ,user starts by selecting the atomic number by using the atomic tab and typing the element symbol in the specified field at the main panel. Closed shell electronic configurations are specified through the "Closed Shells" tab. Initial and final electronic configuration are specified thorough (“Initial Conf” and “Final Conf “) tabs .The user may also restore default data by using the button "default".

After filling the fields with required input data, expected output data has to be selected from the "Print table" menu, which provides four options:

1- Level energy table (lev).
2- Radiative transition rate (table).
3- Mixing coefficients.
4- The wave function (tables).

Then the user clicks "Calculate" button in order to perform the assigned task (see Figure 3.1.1).While HTAC performs the atomic calculation, it displays the massage "wait", which disappears when the task is completed and finally an output file window pops up. HTAC generates four output files with different extensions in separated windows. Output windows are supported with three utilities: print, save and save as that appears in figure (3.2.2). Each file has distinct data. User has the choice to generate one output file for a specific operation or all output files for a particular atom at a very short time. Produced values in output files are reported in atomic units. Other units such as s^{-1} for transition rates and electron volt for energies are also used. However for the purpose of converting the units into one another user may use the known conversion factors. Or can use any suitable unit converter program like Java applet (URL: http://www.pa.uky.edu/~phy211/UnitConverter/index.html).

On the other hand we implement the HTAC during this section to report calculations for energy levels, radiative transition rates, and oscillator strengths for transitions in (O vii) in order to present the validity of HTAC.



```
structure/nombpt/Fe.interpolate.tr
HTAC 1.0.0
Fe Z     =  26.0

NELE     = 10
NTRANS   = 7
MULTIP   = -1
GAUGE    = 2
MODE     = 1
-------------------------------------------------------------------------------------------------
Upper  |  2J  |Lower|2J|   Delta E    |gf(oscillator|Tr(transition|Reduced multipole
       |      |     |  |              |  strengths) |    rate)    |matrix elements
-------------------------------------------------------------------------------------------------
     2  2       0  0  7.258669E+02  1.129517E-01  8.607849E+11   1.127078E-01
     4  2       0  0  7.377441E+02  9.934195E-02  7.820459E+11   1.048454E-01
    16  2       0  0  8.011374E+02  9.463419E-03  8.785168E+10  -3.105322E-02
    22  2       0  0  8.113269E+02  6.222843E-01  5.924731E+12  -2.502261E-01
    26  2       0  0  8.252721E+02  2.493449E+00  2.456309E+13   4.966355E-01
    30  2       0  0  8.941467E+02  3.203146E-02  3.704097E+11   5.407792E-02
    32  2       0  0  8.984370E+02  2.653631E-01  3.098160E+12  -1.552789E-01
Save   Save as   Print
```

Figure 3.2.2. The window of the output file “radiative transition rates table” for the Iron atom (Fe, Z=26).

In Table 3.2.2 and table 3.2.3., we compare the calculated data for energy levels and radiative transition rates for the electric dipole transitions (E1) from HTAC, with the experimental values compiled by **NIST.** However, another comparison with theoretical data was performed with the Super Structure (SS) program. The (SS code and NIST) data are from reference (Aggarwal and Keenan 2008). Generally all HTAC energy levels and transition rates are in a good agreement with SS code and the NIST database values.

Transition Level		**NIST**	**HTAC_CIM**	**HTAC_MBPT**	**SS Code**	
Lower	**Upper**					
1	7	3.309 + 12	3.4736+12	3.4626+ 12	3.403 + 12	
2	3	7.797 + 07	7.837 + 07	7.940 + 07	8.058 + 07	
2	5	8.033 + 07	8.0905+07	8.1802+07	8.309 + 07	
5	8	1.249 + 10	1.297 + 10	1.262 + 10	1.131 + 10	

Table 3.2.2 Comparison of HTAC radiative transition rates (in s^{-1}) for some transitions of O VII.

INDEX	Non-Relativistic Configuration	ENERGY LEVEL			
		NIST	HTAC_CIM	HTAC-MBPT	SS-code
1	$1s^2$	0.00000	0.00000000	0.0000000	0.00000
2	$1s^1\ 2s^1$	41.23155	41.15145	41.15315	41.2438
3	$1s^1\ 2p^1$	41.78724	41.73946	41.70903	41.7933
4	$1s^1\ 2p^1$	41.78779	41.74001	41.71470	41.7942
5	$1s^1\ 2p^1$	41.79280	41.74482	41.71581	41.7997
6	$1s^1\ 2s^1$	41.81240	41.77862	41.72003	41.8074
7	$1s^1\ 2p^1$	42.18438	42.17263	42.12810	42.2100
8	$1s^1\ 3s^1$	48.65091	48.73321	48.53976	48.6577
9	$1s^1\ 3p^1$	48.80446	48.73343	48.69706	48.8114
10	$1s^1\ 3p^1$	48.80446	48.73489	48.69730	48.8116
11	$1s^1\ 3p^1$	48.80446	48.7392	48.69878	48.8132
12	$1s^1\ 3s^1$	48.81129	48.8043	48.70543	48.8217
13	$1s^1\ 3d^1$	48.88374	48.80439	48.76445	48.8930
14	$1s^1\ 3d^1$	48.88428	48.80482	48.76453	48.8931
15	$1s^1\ 3d^1$	48.88437	48.80979	48.76497	48.8935
16	$1s^1\ 3d^1$	48.89376	48.73321	48.76887	48.8971
17	$1s^1\ 3p^1$	48.92183	48.85139	48.81367	48.9281
18	$1s^1\ 4s^1$	51.17986	51.08938	51.05002	51.1813
19	$1s^1\ 4p^1$	51.23690	51.14650	51.10748	51.2436
20	$1s^1\ 4p^1$	51.23690	51.14660	51.10759	51.2437
21	$1s^1\ 4p^1$	51.23690	51.14723	51.10822	51.2444
22	$1s^1\ 4s^1$	51.24146	51.15486	51.11671	51.2475
23	$1s^1\ 4d^1$	51.26752	51.19102	51.15085	51.2767
24	$1s^1\ 4d^1$	51.26788	51.19106	51.15088	51.2767
25	$1s^1\ 4d^1$	51.27244	51.19121	51.15104	51.2769
26	$1s^1\ 4f^1$	0	51.18460	51.14408	51.2786
27	$1s^1\ 4f^1$	0	51.18464	51.14413	51.2785
28	$1s^1\ 4f^1$	51.26980	51.18476	51.14425	51.2787
29	$1s^1\ 4f^1$	51.27554	51.18482	51.14430	51.2787
30	$1s^1\ 4d^1$	51.27399	51.19393	51.15321	51.2790
31	$1s^1\ 4p^1$	51.28702	51.19494	51.15551	51.2916
32	$1s^1\ 5s^1$	52.33051	52.23846	52.19842	0
33	$1s^1\ 5p^1$	52.35630	52.26666	52.22680	0
34	$1s^1\ 5p^1$	52.35630	52.26671	52.22686	0
35	$1s^1\ 5p^1$	52.35630	52.26703	52.22717	0
36	$1s^1\ 5s^1$	0	52.27124	52.23181	0
37	$1s^1\ 5d^1$	52.37416	52.29509	52.25471	0
38	$1s^1\ 5d^1$	52.37435	52.29511	52.25473	0
39	$1s^1\ 5d^1$	52.37617	52.29518	52.25480	0
40	$1s^1\ 5f^1$	0	52.28884	52.24827	0
41	$1s^1\ 5f^1$	0	52.28885	52.24835	0
42	$1s^1\ 5f^1$	52.37234	52.28891	52.24838	0
43	$1s^1\ 5f^1$	52.37799	52.28895	52.24827	0
44	$1s^1\ 5g^1$	0	52.28881	52.24824	0
45	$1s^1\ 5g^1$	0	52.28882	52.24825	0
46	$1s^1\ 5g^1$	0	52.28888	52.24829	0
47	$1s^1\ 5g^1$	0	52.28891	52.24830	0

48	$1s^1 5d^1$	52.38173	52.29518	52.25603	0
49	$1s^1 5p^1$	52.38373	52.29111	52.25109	0

Table3.2.3: Energy levels (in Ryd) for OVII. Zeros in the table means that the values are not available.

3.3. The "option" Tab

Using the "option" tab provides more flexibility to the present GUI In terms of user interface layout because most software make all commands available all the time, which extensively increases the amount of screen space dedicated to interface components such as menus, toolbars and palettes. This quickly becomes a problem in most software as users often want to maximize the space available for the artifacts they are working on (e.g. an image or a text document). HTAC Main screen does not make all command available all the time while using the "option" tab enables accessing many parameters that determine the accuracy of the calculations and make use to all PFAC functions. This bar allows user to switch between the two methods of calculation in order to obtain atomic data and store them in four different output files under different extensions. Pressing the "Option" tab, adds two bars to the main panel of the atomic structure program; the general tab and set transition tab (see Figure 3.1.1). Next section will cover the most important services that provided by these two tabs .The remaining services are described in the HTAC manual.

3.3.1. The General Tab

The user may switch the method of calculation from the (CIM) to (MBPT) by using the "structure menu" from the 'general tab" panel (see figure 3.3.1). The Structure menu has four options each option has a distinctive structure function that generates four output files that has been mentioned above. Output files generated by the two computational methods are saved with different extensions. In the MBPT only single or double excitation are considered in the perturbation expansion. There are two options to indicate whether only single excitation or double excitation is included. Atomic structure program generates four output files for single excitation, double excitation, and combined single excitation and double excitation. If the "singledouble" option in the structure menu is selected, both single and double excitations will be included in the output file .finally HTAC follows the CIM approach in performing atomic calculations by selecting the option CIM.

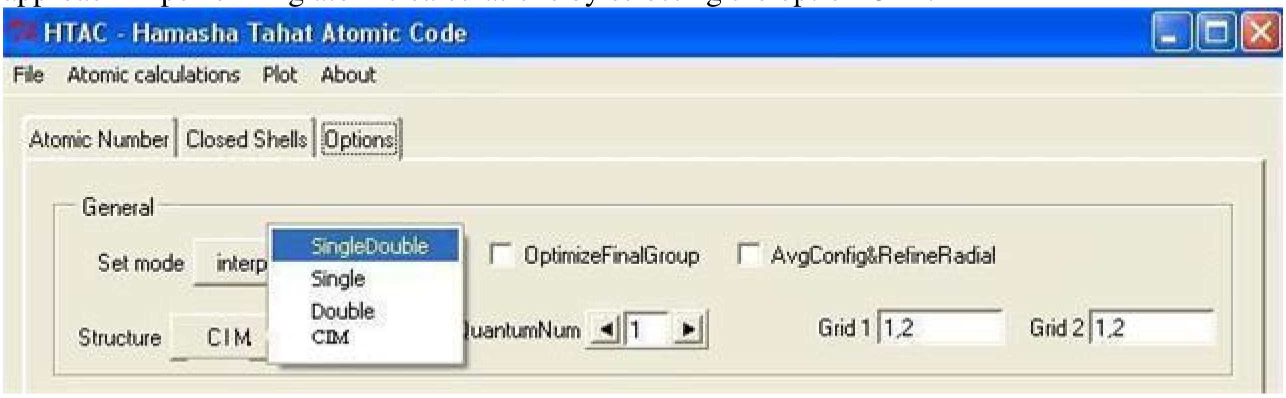


Figure 3.3.1: the General tab.

3.3.2. The "Set Transition "Tab

The set transition tab is used in order to select the radiative transition calculation parameters. (See Figure 3.3.2.) .The following section describes the most important items in this tab and they are:

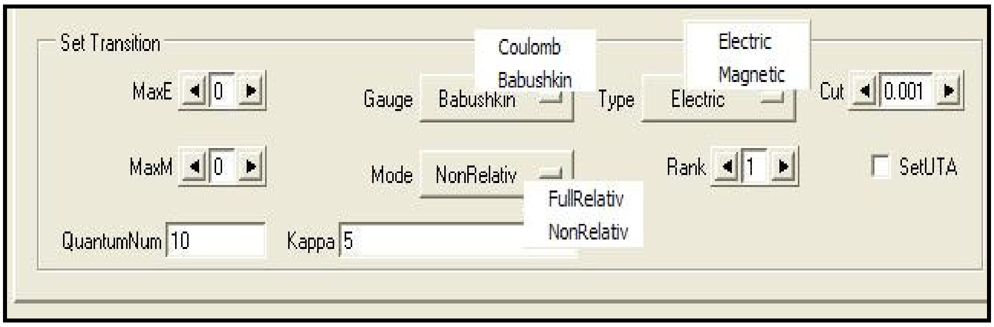


Figure 3.3.2. The “set transition“ tab.

1. Gauge menu: One of the general criteria to assess the accuracy of radiative transition rate is to compare the length and velocity forms of the oscillator strength and transition rates. Table 3.3.1 presents such comparison for some transitions of He like O, generated by using The “Gauge menu” which allows user to set the gauge for radiative transitions. It consists of two options: Babuskin (length form) which is the default option and coulomb (velocity form). Changing the gauge generates new transition table with data for the oscillator strength, transition rates, and the multipoles reduced matrix elements.

Upper	**Lower**	**Babushkin (The length form) HTAC**		**Coulomb (The velocity form) HTAC**	
		Oscillator Strengths gf	**Transition rate tr**	**Oscillator Strengths gf**	**Transition rate tr**
1	0	3.149599-02	8.388378+07	3.149572-02	8.388305+07
2	0	9.454984-02	8.397246+07	9.454966-02	8.397230+07
3	0	1.590494-01	8.612316+07	1.590513-01	8.612420+07
4	2	6.039258-07	6.890124+00	6.041551-07	6.892741+00
5	0	1.959215-05	5.740549+04	1.962878-05	5.751283+04
5	4	7.103952-02	3.557510+07	7.103978-02	3.557523+07

Table 3.3.1 comparison of radiative rates (in s^{-1}), gf (dimensionless) for some transitions of OVII by using HTAC_CIM in the length and velocity forms.

From the compression we noted that there is a good agreement between the length and velocity forms of the gf values for strong transitions; however, for the weak transitions this assessment of accuracy does not apply. But differences between the two forms can sometimes be important even for some very strong transitions, as demonstrated through various examples by (Aggarwal et al., 2007).

2. The "mode" menu: allows user to set the mode for the multipole integral. The menu list consists of two options: a fully relativistic (default) and a non-relativistic approximation. Changing the mode generates new transition table with different values for the oscillator strength, transition rates, and the multipoles reduced matrix elements.
3. “Type” menu: allows user to set the type of multipole. The menu list consists of two options: magnetic and electric. Electric option for the electric multipole transitions (E) implies that the field rank is negative, while the magnetic option implies that the field rank is positive. "multip=" -1, -2, -3 for E1, E2, and E3 transitions and so on respectively, while "multip=" 1, 2, 3 for M1, M2, and M3 transitions respectively. We run this counter from 1 to 99.

4. "Rrank" updownbox : sets the multipole type of transition. We run this counter from 1 to 99. Where dipoles=1, quadrupole =2, octupoles=3, hexadecapole =4, triakontadipole=5, hexacontatetrapole=6, etc.
5. (SetUTA) checkbox: allows adding additional fields into the transition rate table. Pointing it means including the Unresolved Transition Array model in the calculations then the calculations will be carried out in the configuration average approximation and the radiative transition rates output file will contain three additional fields, the transition energy including the UTA shift, the Gausian standard deviation, and the correction to the line strengths due to the configuration interaction within the same non-relativistic configurations.

3.4. Plotting Capabilities

HTAC used Biggles (http://biggles.sourceforge.net/.) to create the graphs, where Biggles is high-level scientific plotting module for creating publication-quality 2D scientific plots works for python programming language. HTAC provides a series of graphs to illustrate the atomic data that has been tabulated in the output files by following the method of calculation. HTAC extracts the required input data automatically for plotting task by selecting one graph from the plot menu. See figure (3.4.1, 3.4.2). HTAC manual provides more details.

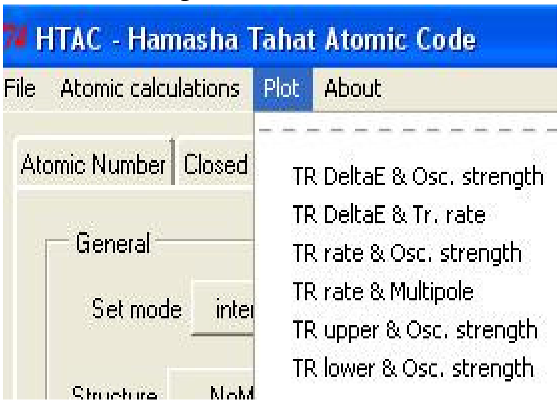


Figure 3.4.1 HTAC "plot" menu

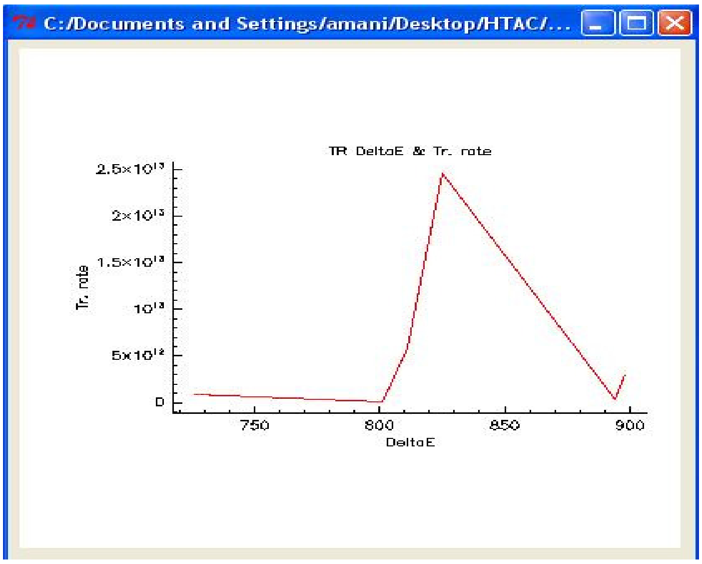


Figure 3.4.2. User can generate this graph by selecting the item (TR DeltaE &Tr.rate) from the plot menu. After calculating the radiative transition rate table for ne like iron.

3.5. Error Massages

One of the most problems with the most atomic codes is that it isn't very vocal about problems it encounters, it will either give results or it won't. Some programs generate same warning massage for all kinds of problems, which may interrupt user. By using HTAC user can get error massages window that describes the error in details so he may determine his mistake then continue working safely. Figure 3.5.1 presents an example of such errors in the background function.

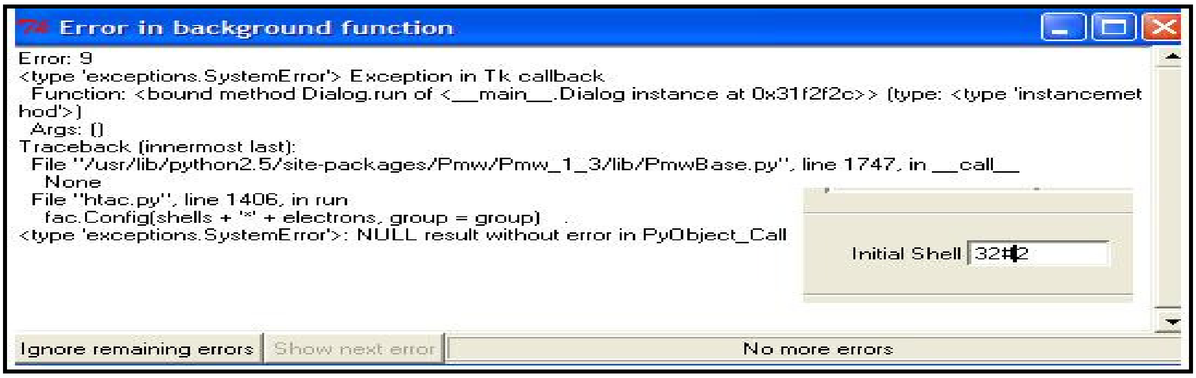


Figure 3.5.1. An error massage window in the background function pops up if user inserts wrong form for the initial shell.

.

The error window can scan for existing errors and has two options:

- Ignore remaining errors: if user choose this option then HTAC will ignore the remaining errors by closing the error massage window ,this will return the user to the main panel, however , user may correct the error in the input file in order to generate the specified output file.
- Show next error: HTAC will continue showing the errors until there are no more errors**.**

3.6. Future Work of HTAC

The goals of the future work are:

1. Adding the “collissional excitation” model of the FAC package , the R _MATRIX (Berrington et al., 1995) code to the HTAC package in order to calculate the (energy levels, collisional excitation, collisonal strength, magnetic sublevel, cross sections of electron impact excitation and the rate coefficients) tables .
2. Implementing the Extended Frequency Dependent Quadrature Rules (EFDQR) (Ixaru et al., 2006) in order to fast the R-matrix method process in calculating the collisional strength.
3. Developing hydrogen like model by assuming only one electron n1 in the system that has an effective charge state to calculate the energy levels, radiative transition rates, and oscillator strength beside some other important atomic data for all h like ions.

3.7. Summary and Conclusion

We have successfully developed an atomic multiplet code for calculating atomic processes (HTAC). In this work we designed, wrote and examined the atomic structure program of the HTAC code, which is one of the programs in this utility program. Two methods for atomic structure calculation have been used in HTAC; the configuration interaction method (CIM) in a fully relativistic approach, and the many body perturbation theory approach (MBPT). Our work consisted in writing the graphical user interface and implementing the procedures that allow a rapid processing and viewing of the calculated atomic data and parameters used in the calculations. HTAC gives access to many parameters that determine the accuracy of the calculations; the program atomic structure allows inputting the parameters through a user friendly interface however ,HTAC makes it easy to specify the input and schedule the computation processes, viewing and plotting capabilities of the atomic data, and therefore, allows typical calculations to be carried out with minimal understanding of theoretical atomic physics .Atomic structure program generates four different output files to the same input data file which are saved with four different extensions relating to the computational method that have been used in generating them. If the user makes any mistake and to continue working safely, many error massages appear in the error background function window. The accuracy of HTAC is checked. Some of the data were compared with some similar data in the literature.

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